Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 01:49 PM EDT

PDB ID	:	2R47
Title	:	Crystal structure of MTH_862 protein of unknown function from Methanothermobacter thermautotrophicus
Authors	:	Osipiuk, J.; Evdokimova, E.; Kudritska, M.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2007-08-30
Resolution	:	1.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

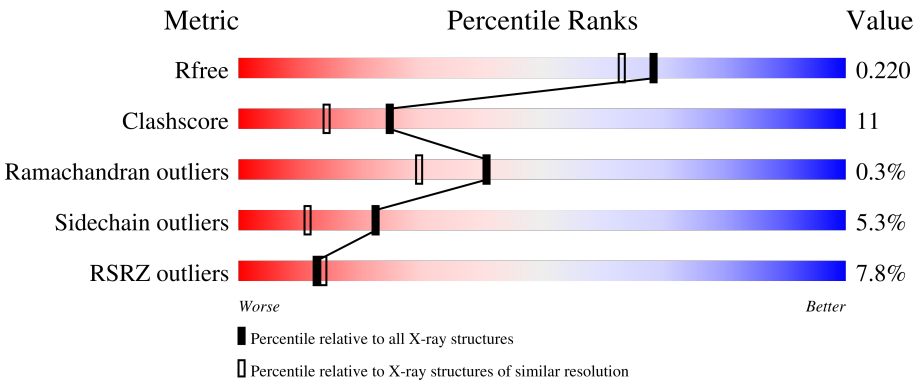
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	157	6% 84% 12%
1	B	157	4% 78% 17%
1	C	157	4% 84% 14%
1	D	157	15% 75% 20%
1	E	157	10% 74% 21%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6896 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Uncharacterized protein MTH_862.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	155	1291	831	206	245	9	0	15	0
1	B	155	1310	843	203	255	9	0	18	0
1	C	155	1282	823	202	249	8	0	14	0
1	D	153	1235	791	198	238	8	0	6	0
1	E	155	1247	795	203	241	8	0	8	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP O26950
A	0	HIS	-	EXPRESSION TAG	UNP O26950
A	154	GLY	-	EXPRESSION TAG	UNP O26950
A	155	SER	-	EXPRESSION TAG	UNP O26950
B	-1	GLY	-	EXPRESSION TAG	UNP O26950
B	0	HIS	-	EXPRESSION TAG	UNP O26950
B	154	GLY	-	EXPRESSION TAG	UNP O26950
B	155	SER	-	EXPRESSION TAG	UNP O26950
C	-1	GLY	-	EXPRESSION TAG	UNP O26950
C	0	HIS	-	EXPRESSION TAG	UNP O26950
C	154	GLY	-	EXPRESSION TAG	UNP O26950
C	155	SER	-	EXPRESSION TAG	UNP O26950
D	-1	GLY	-	EXPRESSION TAG	UNP O26950
D	0	HIS	-	EXPRESSION TAG	UNP O26950
D	154	GLY	-	EXPRESSION TAG	UNP O26950
D	155	SER	-	EXPRESSION TAG	UNP O26950
E	-1	GLY	-	EXPRESSION TAG	UNP O26950
E	0	HIS	-	EXPRESSION TAG	UNP O26950
E	154	GLY	-	EXPRESSION TAG	UNP O26950

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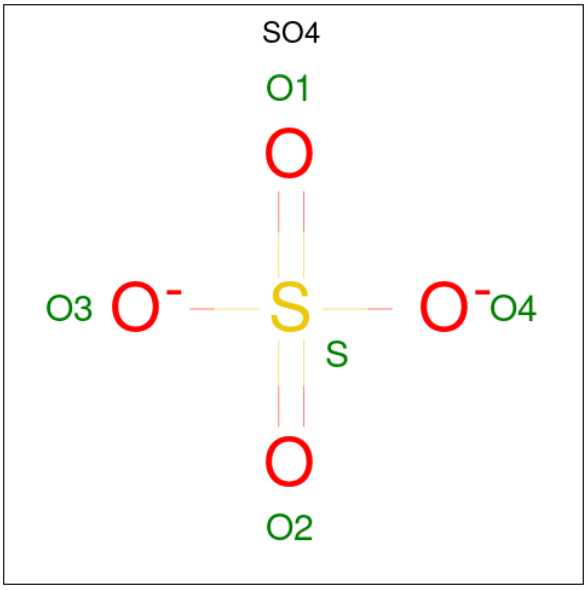
Chain	Residue	Modelled	Actual	Comment	Reference
E	155	SER	-	EXPRESSION TAG	UNP O26950

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	132	134	134	0	3
3	B	127	130	130	0	4
3	C	118	119	119	0	1
3	D	57	57	57	0	1

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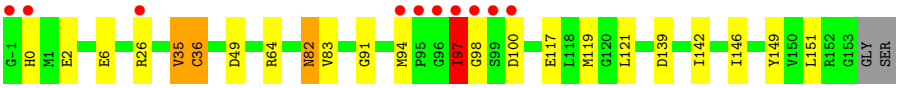
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	E	65	66	66	0	1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

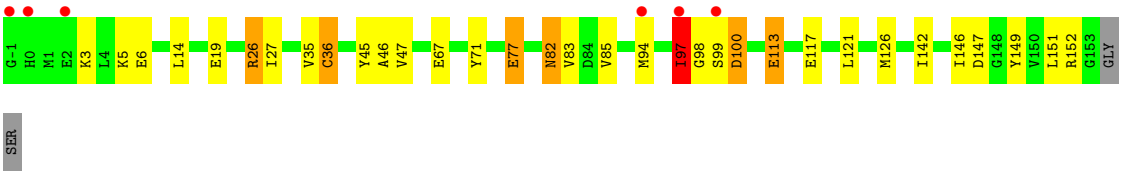
• Molecule 1: Uncharacterized protein MTH_862

Chain A:



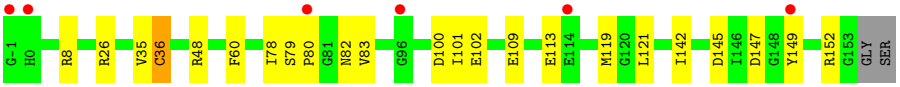
• Molecule 1: Uncharacterized protein MTH_862

Chain B:



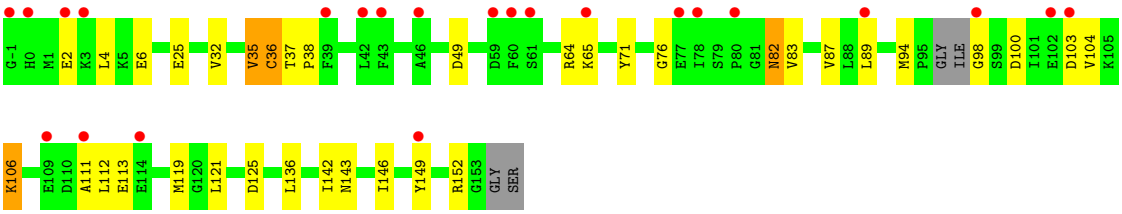
• Molecule 1: Uncharacterized protein MTH_862

Chain C:



• Molecule 1: Uncharacterized protein MTH_862

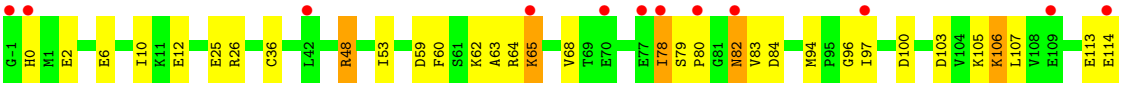
Chain D:

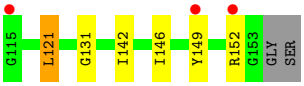


• Molecule 1: Uncharacterized protein MTH_862

Chain E:

10%
74%
21%


G-1
H0
M1
E2
E6
I10
K11
E12
E25
R26
C36
L42
R48
I53
D59
F60
S61
K62
A63
R64
K65
V68
T69
E70
E77
I78
S79
P80
G81
N82
V83
D84
M94
P95
G96
I97
D100
D103
V104
K105
K106
L107
V108
E109
E113
E114


G115
L121
G131
I142
I146
Y149
R152
G153
GLY
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	150.76Å 208.64Å 83.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.80 – 1.88 34.70 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.80-1.88) 99.4 (34.70-1.88)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 1.88Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.221 0.192 , 0.220	Depositor DCC
R_{free} test set	5306 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6896	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, OCS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.80	0/1344	0.84	0/1803
1	B	0.88	2/1377 (0.1%)	0.85	1/1851 (0.1%)
1	C	0.82	0/1332	0.84	0/1789
1	D	0.81	2/1259 (0.2%)	0.71	1/1692 (0.1%)
1	E	0.72	0/1276	0.76	1/1713 (0.1%)
All	All	0.81	4/6588 (0.1%)	0.80	3/8848 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	1	1
All	All	1	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	106	LYS	CE-NZ	10.95	1.76	1.49
1	D	106	LYS	CD-CE	10.51	1.77	1.51
1	B	113	GLU	CB-CG	-7.18	1.38	1.52
1	B	85	VAL	CB-CG1	5.17	1.63	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	121	LEU	CA-CB-CG	6.32	129.85	115.30
1	B	97	ILE	CB-CA-C	6.17	123.95	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	106	LYS	CG-CD-CE	-5.61	95.08	111.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	97	ILE	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	ILE	Peptide
1	B	97	ILE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1291	0	1304	33	0
1	B	1310	0	1315	35	0
1	C	1282	0	1278	18	2
1	D	1235	0	1215	29	0
1	E	1247	0	1234	49	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
3	A	134	0	0	6	0
3	B	130	0	0	8	0
3	C	119	0	0	4	1
3	D	57	0	0	1	0
3	E	66	0	0	5	0
All	All	6896	0	6346	137	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:LYS:CD	1:D:106:LYS:CE	1.77	1.58
1:D:106:LYS:CE	1:D:106:LYS:NZ	1.76	1.47
1:B:117[A]:GLU:HB2	3:B:830[A]:HOH:O	1.15	1.30
1:E:59:ASP:HB3	1:E:62:LYS:NZ	1.47	1.26
1:B:94[B]:MET:HG3	1:B:126:MET:HE1	1.21	1.13
1:A:146:ILE:HD12	1:B:146:ILE:HD13	1.37	1.06
1:B:97:ILE:HA	1:B:98:GLY:O	1.55	1.05
1:E:65:LYS:NZ	1:E:79:SER:HB3	1.72	1.04
1:A:146:ILE:CD1	1:B:146:ILE:HD13	1.91	1.01
1:E:59:ASP:HB3	1:E:62:LYS:HZ3	0.96	0.98
1:C:119:MET:SD	3:C:760:HOH:O	2.21	0.96
1:E:59:ASP:CB	1:E:62:LYS:NZ	2.32	0.93
1:E:48:ARG:HG3	1:E:48:ARG:HH11	1.33	0.92
1:A:97:ILE:HA	1:A:98:GLY:O	1.70	0.91
1:D:106:LYS:CE	1:D:106:LYS:CG	2.49	0.90
1:A:146:ILE:HD12	1:B:146:ILE:CD1	2.01	0.90
1:E:59:ASP:CB	1:E:62:LYS:HZ3	1.82	0.90
1:A:146:ILE:CD1	1:B:146:ILE:CD1	2.52	0.87
1:E:82:ASN:ND2	1:E:113:GLU:HG2	1.89	0.87
1:C:8[A]:ARG:HG3	1:C:8[A]:ARG:HH11	1.40	0.87
1:C:152[A]:ARG:HD3	3:C:790:HOH:O	1.74	0.87
1:B:94[B]:MET:CG	1:B:126:MET:HE1	2.06	0.83
1:D:125:ASP:H	1:D:143:ASN:HD21	1.25	0.82
1:E:65:LYS:CE	1:E:79:SER:HB3	2.10	0.80
1:E:82:ASN:HD22	1:E:113:GLU:HG2	1.46	0.80
1:E:65:LYS:HZ2	1:E:79:SER:HB3	1.44	0.79
1:A:26[A]:ARG:HG3	3:A:810:HOH:O	1.83	0.79
1:B:94[B]:MET:HG3	1:B:126:MET:CE	2.11	0.76
1:E:59:ASP:HB3	1:E:62:LYS:HZ1	1.49	0.74
1:A:35[B]:VAL:HG23	1:A:36:OCS:OD3	1.87	0.73
1:B:67[A]:GLU:OE2	3:B:809:HOH:O	2.06	0.73
1:D:83:VAL:O	1:D:113:GLU:HG3	1.87	0.73
1:D:146[B]:ILE:CD1	1:E:146:ILE:HD12	2.21	0.71
1:E:83:VAL:O	1:E:113:GLU:HG3	1.90	0.70
1:A:26[A]:ARG:CG	3:A:810:HOH:O	2.39	0.70
1:A:35[B]:VAL:CG2	1:A:36:OCS:OD3	2.40	0.70
1:E:48:ARG:HB2	1:E:68:VAL:HG21	1.76	0.68
1:B:97:ILE:CA	1:B:98:GLY:O	2.40	0.65
1:D:4:LEU:HD22	1:E:152[A]:ARG:NH1	2.12	0.65
1:D:146[B]:ILE:CD1	1:E:146:ILE:CD1	2.75	0.64
1:D:125:ASP:H	1:D:143:ASN:ND2	1.93	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LEU:HD12	1:A:142:ILE:HB	1.79	0.64
3:A:729:HOH:O	1:D:49:ASP:HB3	1.99	0.63
1:A:97:ILE:CA	1:A:98:GLY:O	2.46	0.62
1:D:146[B]:ILE:HD12	1:E:146:ILE:CD1	2.28	0.62
1:E:48:ARG:HG3	1:E:48:ARG:NH1	2.09	0.62
1:B:26:ARG:NH1	1:B:113:GLU:OE2	2.30	0.62
1:A:6:GLU:HG2	1:B:149[A]:TYR:CE1	2.35	0.62
1:C:78:ILE:HG22	1:C:80:PRO:HD3	1.81	0.62
1:E:59:ASP:CB	1:E:62:LYS:HZ1	2.07	0.61
1:C:8[A]:ARG:HG3	1:C:8[A]:ARG:NH1	2.14	0.61
1:B:100:ASP:HB2	3:B:769:HOH:O	2.01	0.61
1:A:149[B]:TYR:CD1	1:A:151:LEU:HD11	2.36	0.60
1:A:149[B]:TYR:CE1	1:A:151:LEU:HD11	2.37	0.60
1:C:35[B]:VAL:HG23	1:C:36:OCS:OD3	2.01	0.60
1:E:65:LYS:HE3	1:E:79:SER:HB3	1.83	0.60
1:C:109[B]:GLU:HA	1:C:109[B]:GLU:OE2	2.02	0.60
1:E:0:HIS:HE1	1:E:2[B]:GLU:OE2	1.85	0.59
1:B:77[A]:GLU:HG3	3:B:727:HOH:O	2.03	0.59
1:D:100:ASP:HB3	1:D:103:ASP:OD1	2.03	0.59
1:B:121:LEU:HD12	1:B:142:ILE:HB	1.82	0.59
1:E:107:LEU:HA	3:E:755:HOH:O	2.02	0.58
1:E:59:ASP:CG	1:E:62:LYS:HZ1	2.08	0.57
1:A:26[A]:ARG:HG2	1:A:83:VAL:HG12	1.88	0.55
1:A:94[A]:MET:SD	1:E:97:ILE:HG13	2.46	0.55
1:E:65:LYS:HZ2	1:E:79:SER:CB	2.18	0.55
1:A:64[B]:ARG:HD2	1:B:71:TYR:CZ	2.42	0.55
1:A:91:GLY:O	1:A:94[A]:MET:HG2	2.07	0.54
1:D:35:VAL:CG2	1:D:36:OCS:OD3	2.55	0.54
1:B:26:ARG:HG3	1:B:83:VAL:HA	1.88	0.54
1:A:97:ILE:C	1:A:98:GLY:O	2.45	0.54
1:A:82:ASN:HD22	1:A:82:ASN:C	2.11	0.53
1:E:65:LYS:HZ1	1:E:79:SER:HB3	1.71	0.53
1:E:106:LYS:HG2	3:E:755:HOH:O	2.08	0.53
1:D:87:VAL:HG22	1:D:119:MET:HE2	1.91	0.53
1:D:35:VAL:HG22	1:D:36:OCS:OD3	2.09	0.52
1:D:71:TYR:CE1	1:E:64:ARG:HD3	2.43	0.52
1:A:97:ILE:HD12	3:D:748:HOH:O	2.10	0.52
1:A:6:GLU:HG2	1:B:149[A]:TYR:CD1	2.44	0.52
1:C:121[A]:LEU:HD23	1:C:142:ILE:HB	1.91	0.52
1:A:97:ILE:HG22	3:A:814:HOH:O	2.10	0.52
1:B:117[B]:GLU:HG2	3:B:830[B]:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ILE:HG22	3:B:734:HOH:O	2.10	0.51
1:D:146[A]:ILE:CD1	1:E:10:ILE:HD13	2.41	0.51
1:E:103:ASP:O	1:E:106:LYS:HD3	2.10	0.51
1:D:106:LYS:CE	1:D:106:LYS:HG2	2.41	0.50
1:E:80:PRO:HD3	3:E:738:HOH:O	2.12	0.50
1:A:49:ASP:HB2	1:C:102:GLU:HG2	1.93	0.50
1:D:149[A]:TYR:CD1	1:E:6:GLU:HG2	2.47	0.50
1:D:94:MET:O	1:D:98:GLY:HA3	2.12	0.50
1:C:82:ASN:HB3	1:C:113[B]:GLU:HG3	1.93	0.49
1:C:48:ARG:HD2	3:C:775:HOH:O	2.12	0.49
1:D:121:LEU:HD23	1:D:142:ILE:HB	1.95	0.49
1:E:12:GLU:HG3	3:E:709:HOH:O	2.13	0.48
1:A:149[A]:TYR:CE1	1:B:6[A]:GLU:HG2	2.49	0.48
1:C:78:ILE:CG2	1:C:80:PRO:HD3	2.43	0.48
1:D:71:TYR:CZ	1:E:64:ARG:HD3	2.49	0.47
1:A:97:ILE:O	1:E:97:ILE:HD11	2.15	0.47
1:D:4:LEU:HD22	1:E:152[B]:ARG:HE	1.80	0.47
1:A:117[A]:GLU:HG3	1:A:139:ASP:HB2	1.97	0.47
1:D:149[A]:TYR:CE1	1:E:6:GLU:HG2	2.49	0.47
1:B:26:ARG:NH2	1:B:113:GLU:OE2	2.50	0.45
1:C:26:ARG:HD3	1:C:82:ASN:O	2.15	0.45
1:C:152[A]:ARG:NH1	3:C:790:HOH:O	2.48	0.45
1:A:146:ILE:HD13	1:B:146:ILE:HD13	1.91	0.45
1:D:146[B]:ILE:HD13	1:E:146:ILE:HD12	1.98	0.45
1:B:35:VAL:HG13	1:B:36:OCS:OD3	2.17	0.44
1:B:97:ILE:HG23	3:B:813:HOH:O	2.17	0.44
1:B:149[B]:TYR:CD2	1:B:151:LEU:HD11	2.52	0.44
1:A:35[A]:VAL:HB	1:A:36:OCS:OD3	2.18	0.44
1:B:97:ILE:C	1:B:98:GLY:O	2.55	0.43
1:E:121:LEU:HD23	1:E:142:ILE:HB	1.99	0.43
1:C:60:PHE:O	1:C:80:PRO:HB3	2.18	0.43
1:E:82:ASN:HD22	1:E:113:GLU:CG	2.25	0.43
1:E:53:ILE:HD12	1:E:63:ALA:HB1	2.01	0.43
1:B:5:LYS:HD2	3:B:786:HOH:O	2.17	0.43
1:C:8[A]:ARG:NH1	1:C:8[A]:ARG:CG	2.82	0.43
1:D:82:ASN:HB2	1:D:111:ALA:O	2.19	0.43
1:E:78:ILE:H	1:E:78:ILE:HG12	1.58	0.42
1:B:14:LEU:HD22	1:B:46:ALA:HB2	2.02	0.42
1:E:60:PHE:O	1:E:80:PRO:HB3	2.20	0.42
3:A:824:HOH:O	1:C:101:ILE:HG21	2.19	0.42
1:B:27[A]:ILE:HD12	1:B:47:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117[A]:GLU:HG2	1:A:119:MET:HG3	2.00	0.41
1:A:94[A]:MET:SD	1:E:97:ILE:CG1	3.08	0.41
1:C:26:ARG:HG2	1:C:83:VAL:HG12	2.02	0.41
1:A:0:HIS:HE1	1:A:2:GLU:OE1	2.04	0.41
1:D:64:ARG:HD3	1:D:76:GLY:O	2.21	0.41
1:B:19:GLU:OE2	1:E:131:GLY:HA2	2.22	0.40
1:D:37:THR:HB	1:D:38:PRO:HD3	2.02	0.40
1:E:94:MET:HG3	3:E:746:HOH:O	2.21	0.40
1:A:100:ASP:CG	3:A:729:HOH:O	2.60	0.40
1:D:6:GLU:HG2	1:E:149:TYR:CD1	2.56	0.40
1:B:45:TYR:OH	1:E:96:GLY:HA2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147[B]:ASP:OD1	3:C:767:HOH:O[3_555]	2.16	0.04
1:C:145:ASP:OD2	1:C:149[B]:TYR:OH[3_555]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	166/157 (106%)	159 (96%)	6 (4%)	1 (1%)	25 14
1	B	170/157 (108%)	166 (98%)	3 (2%)	1 (1%)	25 14
1	C	165/157 (105%)	161 (98%)	4 (2%)	0	100 100
1	D	154/157 (98%)	150 (97%)	4 (3%)	0	100 100
1	E	158/157 (101%)	149 (94%)	9 (6%)	0	100 100
All	All	813/785 (104%)	785 (97%)	26 (3%)	2 (0%)	41 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	ILE
1	B	97	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	138/125 (110%)	135 (98%)	3 (2%)	52	43
1	B	142/125 (114%)	130 (92%)	12 (8%)	10	3
1	C	137/125 (110%)	135 (98%)	2 (2%)	65	59
1	D	129/125 (103%)	116 (90%)	13 (10%)	7	2
1	E	130/125 (104%)	120 (92%)	10 (8%)	13	4
All	All	676/625 (108%)	636 (94%)	40 (6%)	22	9

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35[A]	VAL
1	A	35[B]	VAL
1	A	82	ASN
1	B	3	LYS
1	B	26	ARG
1	B	77[A]	GLU
1	B	77[B]	GLU
1	B	82[A]	ASN
1	B	82[B]	ASN
1	B	99	SER
1	B	100	ASP
1	B	147[A]	ASP
1	B	147[B]	ASP
1	B	152[A]	ARG
1	B	152[B]	ARG
1	C	79	SER

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Mol	Chain	Res	Type
1	C	100	ASP
1	D	2[A]	GLU
1	D	2[B]	GLU
1	D	25	GLU
1	D	32	VAL
1	D	35	VAL
1	D	65	LYS
1	D	82	ASN
1	D	89	LEU
1	D	104	VAL
1	D	112	LEU
1	D	136	LEU
1	D	152[A]	ARG
1	D	152[B]	ARG
1	E	25	GLU
1	E	48	ARG
1	E	65	LYS
1	E	78	ILE
1	E	82	ASN
1	E	84	ASP
1	E	100	ASP
1	E	105	LYS
1	E	106	LYS
1	E	114	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	82	ASN
1	B	0	HIS
1	B	41	GLN
1	B	52	ASN
1	D	82	ASN
1	D	143	ASN
1	E	0	HIS
1	E	52	ASN
1	E	82	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OCS	C	36	1	6,8,9	1.76	2 (33%)	7,11,13	1.65	1 (14%)
1	OCS	D	36	1	6,8,9	1.16	0	7,11,13	1.00	1 (14%)
1	OCS	B	36	1	6,8,9	1.91	1 (16%)	7,11,13	1.10	1 (14%)
1	OCS	A	36	1	6,8,9	1.68	1 (16%)	7,11,13	1.08	0
1	OCS	E	36	1	6,8,9	1.37	1 (16%)	7,11,13	1.37	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	C	36	1	-	0/4/7/9	-
1	OCS	D	36	1	-	0/4/7/9	-
1	OCS	B	36	1	-	0/4/7/9	-
1	OCS	A	36	1	-	0/4/7/9	-
1	OCS	E	36	1	-	0/4/7/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	OCS	OD3-SG	-4.27	1.33	1.45
1	A	36	OCS	OD3-SG	-3.63	1.34	1.45
1	C	36	OCS	OD3-SG	-3.14	1.36	1.45
1	C	36	OCS	CB-CA	-2.62	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	36	OCS	OD3-SG	-2.31	1.38	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	36	OCS	OD3-SG-CB	3.72	112.31	106.76
1	E	36	OCS	CA-CB-SG	2.20	116.87	113.61
1	B	36	OCS	OD3-SG-CB	2.13	109.93	106.76
1	D	36	OCS	OD1-SG-CB	2.07	109.85	106.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	36	OCS	1	0
1	D	36	OCS	2	0
1	B	36	OCS	1	0
1	A	36	OCS	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	D	704	-	4,4,4	0.46	0	6,6,6	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	E	705	-	4,4,4	0.16	0	6,6,6	0.44	0
2	SO4	C	703	-	4,4,4	0.67	0	6,6,6	0.53	0
2	SO4	A	701	-	4,4,4	0.56	0	6,6,6	0.58	0
2	SO4	B	702	-	4,4,4	0.26	0	6,6,6	0.71	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	154/157 (98%)	0.24	10 (6%)	18	20	14, 21, 30, 34	0
1	B	154/157 (98%)	0.03	6 (3%)	39	41	13, 21, 29, 37	0
1	C	154/157 (98%)	-0.00	6 (3%)	39	41	14, 22, 32, 35	0
1	D	152/157 (96%)	0.69	23 (15%)	2	2	9, 20, 28, 35	0
1	E	154/157 (98%)	0.64	15 (9%)	7	8	12, 20, 30, 35	0
All	All	768/785 (97%)	0.32	60 (7%)	13	14	9, 21, 30, 37	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94[A]	MET	8.9
1	A	95	PRO	7.4
1	A	96	GLY	6.5
1	D	42	LEU	5.3
1	E	114	GLU	4.9
1	A	97	ILE	4.9
1	A	99	SER	4.8
1	E	78	ILE	4.6
1	D	114[A]	GLU	4.3
1	D	0	HIS	4.1
1	D	61	SER	4.1
1	D	39	PHE	3.9
1	E	115	GLY	3.9
1	E	-1[A]	GLY	3.7
1	E	80	PRO	3.7
1	E	0	HIS	3.7
1	E	97	ILE	3.6
1	B	94[A]	MET	3.6
1	D	98	GLY	3.6
1	D	149[A]	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	98	GLY	3.3
1	D	2[A]	GLU	3.3
1	D	43	PHE	3.2
1	A	-1	GLY	3.1
1	E	109[A]	GLU	3.1
1	C	149[A]	TYR	3.1
1	A	0	HIS	3.1
1	D	-1	GLY	3.1
1	E	77	GLU	3.0
1	D	80	PRO	3.0
1	B	97	ILE	2.9
1	B	0	HIS	2.9
1	D	60	PHE	2.8
1	C	0	HIS	2.7
1	D	77	GLU	2.6
1	C	114	GLU	2.6
1	E	152[A]	ARG	2.6
1	D	3	LYS	2.5
1	C	80	PRO	2.5
1	D	65	LYS	2.5
1	E	149	TYR	2.5
1	E	65	LYS	2.4
1	D	59	ASP	2.4
1	D	89	LEU	2.4
1	E	82	ASN	2.4
1	D	111	ALA	2.3
1	B	99	SER	2.3
1	C	-1	GLY	2.2
1	C	96	GLY	2.2
1	D	46	ALA	2.2
1	B	2[A]	GLU	2.1
1	D	102[A]	GLU	2.1
1	D	103	ASP	2.1
1	A	26[A]	ARG	2.1
1	E	42	LEU	2.1
1	B	-1	GLY	2.1
1	D	109	GLU	2.1
1	D	78	ILE	2.0
1	A	100	ASP	2.0
1	E	70	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OCS	D	36	9/10	0.97	0.09	6,13,14,15	3
1	OCS	B	36	9/10	0.98	0.12	5,13,15,16	3
1	OCS	A	36	9/10	0.98	0.12	4,13,16,16	3
1	OCS	E	36	9/10	0.98	0.18	6,14,15,15	3
1	OCS	C	36	9/10	0.99	0.15	9,17,18,18	3

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	701	5/5	0.93	0.15	31,32,32,32	5
2	SO4	D	704	5/5	0.94	0.14	33,33,36,38	5
2	SO4	C	703	5/5	0.95	0.13	29,30,32,34	5
2	SO4	B	702	5/5	0.95	0.12	33,33,34,35	5
2	SO4	E	705	5/5	0.96	0.12	35,37,38,38	5

6.5 Other polymers (i)

There are no such residues in this entry.